EFFECT OF WIND FLUCTUATIONS ON NEAR-RANGE ATMOSPHERIC DISPERSION UNDER DIFFERENT TYPES OF THERMAL STRATIFICATION

Lieven Vervecken[1,2], Johan Camps[2] and Johan Meyers[1]

[1] SCK•CEN, Belgian Nuclear Research Centre, Boeretang 200, 2400 Mol, Belgium
[2] Department of Mechanical Engineering, KU Leuven, Celestijnenlaan 300, 3000 Leuven, Belgium

Abstract: When using the mean wind direction in Reynolds-averaged Navier−Stokes (RANS) simulations of atmospheric dispersion, it is well documented that peak concentration levels are often overestimated, and lateral spreading underestimated. Recently, it has been illustrated for neutrally stratified boundary layers that simulations improve significantly when the effective variability of wind directions, obtained by reducing the variability observed in experiments with the fluctuations predicted in the RANS turbulence model, is included in the boundary conditions. In the current work, we extend this approach towards thermally stratified boundary layers. We test the approach by performing a series of dispersion simulations of the Project Prairie Grass experiments, and demonstrate that also under these conditions the simulations improve markedly.

Key words: *dispersion; wind fluctuations; Project Prairie Grass; atmospheric boundary layer***.**

INTRODUCTION

Although (semi-)Gaussian models are frequently used to assess atmospheric pollutant dispersion after accidental releases (Thoman et al., 2006), they are known to have a limited accuracy close to the source or in situations with complex air flow (Piringer and Baumann-Stanzer, 2009). In these situations, Computational Fluid Dynamics (CFD) could serve as an alternative.

Regardless the CFD approach applied however, it is important to incorporate effects of variable wind conditions imposed by the atmosphere to obtain good predictions of dispersion. When using only the mean wind direction in Reynolds-averaged Navier−Stokes (RANS) simulations of atmospheric dispersion, a large disagreement between simulations and experimental data is often observed, manifesting as a large overestimation of the maximum concentration and a significant underestimation of the plume spread (e.g. Riddle et al., 2004; Tang et al., 2006; Blocken et al., 2008). A number of studies report that if the variability of wind directions observed in experiments is included in the boundary conditions, peak levels improve, but lateral spreading is overestimated (Huber et al., 2004; Tang et al., 2006). Recently, a new approach has been developed addressing this issue for neutrally stratified atmospheric boundary layers by arguing that fluctuations in wind directions observed in experiments are partly accounted for by the modelled turbulence in RANS simulations (Vervecken et al., 2013). Hence, the effective variability of wind directions that is included in the boundary conditions needs to be reduced by a variability derived from the turbulence levels predicted in the RANS turbulence model (Vervecken et al., 2013).

In the current work, we extend this approach towards thermally stratified boundary layers and we test the approach by performing a series of dispersion simulations of the Project Prairie Grass experiments (Barad, 1958). The pollutant dispersion is modeled using a three-dimensional convection-diffusion problem in which analytical profiles for velocity and eddy viscosity are prescribed as function of height, and in which the turbulent pollutant dispersion is modeled based on an eddy-diffusivity approach.

VARIABILITY OF WIND DIRECTION

Consider a variable wind vector $\mathbf{u}(u,v,w)$, e.g., observed at a meteorological tower. We denote the time-averaged velocity with $\langle\mathbf{u}\rangle = (\langle u\rangle, \langle v\rangle, \langle w\rangle)$, and select the coordinate system such that $\langle v\rangle = \langle w\rangle = 0$, i.e. the x-direction is aligned with the mean-flow direction; further the z-direction is normal to the ground. We define the instantaneous wind direction α as the angle between the prompt wind direction and the mean wind direction, i.e. the angle with the x-direction. As elaborated in Vervecken et al. (2013), the total variance of the wind direction σ_α^2, obtained from experiments, can be decomposed as

$$\sigma_\alpha^2 = \sigma_e^2 + \sigma_m^2 \tag{1}$$

where σ_m^2 is a part of the variance that is internally accounted for by the CFD model, and σ_e^2 needs to be accounted for in the boundary conditions. We will simply estimate σ_m^2 based on a single simulation in which we evaluate the turbulent characteristics at the level of the experimental measurement of wind direction. Next, we weight the solution assuming a normal distribution for the wind direction characterized by a zero mean and the reduced variance.

DISPERSION MODEL FOR PRAIRIE GRASS EXPERIMENTS

We simulate the experiments using a simple advection-diffusion equation. Because of the very simple set-up of the experiments, i.e. a wide open prairie in Nebraska without any obstructions from buildings or vegetation, we simply presume a logarithmic mean velocity profile that is extended to a thermally stratified boundary layer by the Monin-Obukhov similarity theory (Monin and Obukhov, 1954). Accordingly we can write (cf., e.g. Paulson, 1970)

$$\frac{d\langle u\rangle}{dz} = \frac{u_*}{\kappa z}\phi_M \ , \tag{2}$$

with $\kappa \approx 0.40$ the von Kármán constant, z_0 the surface roughness length, $u_* \equiv \sqrt{\tau_w/\rho}$ where τ_w is the wall shear stress and ϕ_M a stability function. Several analytical expression for ϕ_M have been suggested (Businger et al, 1971; Dyer, 1974; Foken, 2006), but among the more frequently used, are the following (cf., e.g. Stull, 1988)

$$\phi_M = \begin{cases} (1-\gamma_1\zeta)^{-0.25} & \text{for} \quad -2 < \zeta < 0 \,(\text{unstable}) \\ 1+\beta\zeta & \text{for} \quad 0 \le \zeta < 1 \,(\text{stable}) \end{cases} \tag{3}$$

where γ_1 and β are model constants and where $\zeta \equiv z/L$ with L the Monin-Obukhov length. In the current work, we assume $\gamma_1 = 16$ and $\beta = 5$ (see, Garrat and Pielke, 1989, for a discussion).

Integration of equation (2) leads to the mean velocity profile (cf., e.g., Stull 1988)

$$\langle u\rangle = \frac{u_*}{\kappa}\left[\ln\left(\frac{z}{z_0}\right) - \psi_M(\zeta)\right] \tag{4}$$

with, if $x = (1-\gamma_1\zeta)^{0.25}$,

$$\psi_M = \begin{cases} \ln\left[\left(\frac{1+x^2}{2}\right)\left(\frac{1+x}{2}\right)^2\right] - 2\tan^{-1}x + \frac{\pi}{2} & \text{for} \quad -2 < \zeta < 0 \,(\text{unstable}) \\ -\beta\zeta & \text{for} \quad 0 \le \zeta < 1 \,(\text{stable}) \end{cases} \tag{5}$$

Values for z_0, u_* and L are obtained from a least-squares fit of the velocity profiles to experimental data, together with a similar fits for the potential temperature (Brunell, 1989).

Given this boundary-layer velocity field, the Reynolds-averaged stationary advection−diffusion equation is solved, which is given by (cf., e.g., Bird et al., 2006)

$$\nabla\cdot(\langle \mathbf{u}\rangle\langle c\rangle) = \nabla\cdot(D\nabla\langle c\rangle - \langle \mathbf{u}'c'\rangle) + \langle S_p\rangle \ , \tag{6}$$

where $\langle c\rangle$ is the mean concentration, $\langle \mathbf{u}\rangle = (\langle u\rangle,0,0)$ is the mean velocity field, D is the molecular diffusivity and $\langle S_p\rangle$ the pollutant source term. We model the turbulent mass flux $\langle \mathbf{u}'c'\rangle$ with an eddy-diffusivity approach, i.e. (cf., e.g., Bird et al., 2006)

$$-\langle \mathbf{u}'c'\rangle \approx \frac{\nu_t}{Sc_t}\nabla\langle c\rangle \ , \tag{7}$$

with Sc_t the turbulent Schmidt number, and ν_t the eddy viscosity. In the current study we employ $Sc_t = 0.9$ (see, e.g., Tominaga and Stathopoulos, 2007; and Vervecken et al., 2013, for a discussion). Because thermal stratification does not influence the x-momentum balance, the development in Vervecken et al. 2013 can be repeated, substituting Eq. (2) for the velocity gradient, to obtain an analytical expression for the eddy-viscosity required in Eq. (7)

$$\nu_t = \frac{u_*\kappa z(1-z/\delta)}{\phi_m} \ , \tag{8}$$

where $\delta = Au_*/f$ (with f the Coriolis parameter, and $A \approx 12$ an empirical constant – cf., e.g., Tennekes and Lumley (1972), for an overview).

Finally, to present results, we normalize the concentration in the current study as

$$C^+ = \langle c\rangle\frac{UL^2}{r} \ , \tag{9}$$

where r is the release rate, U is the mean wind speed at 2 m altitude, and L a characteristic length scale that we set to 100 m (i.e. the distance from the point of release to the second measurement arc at the Prairie Grass Experiments).

COMPUTATIONAL SET-UP

We solve the convection−diffusion problem (6) using the OpenFOAM finite-volume open-source simulation platform for the dispersion simulations of the Project Prairie Grass experiments. All experiments are included in the analysis except for those with insufficient data, with a wind speed lower than 2 ms^{-1} at 2 m altitude, or with $\sigma_\alpha > 17.5$. Identification of the stability class is based on σ_α (cf., e.g., Zanetti, 1990).

For the construction of a solution that is weighted over the different wind directions, we apply the same approach as discussed in Vervecken et al. (2013), i.e. rotating the numerical solution around the vertical axis through the source, while maintaining the sensor locations. A series of angles is taken over the range of $\left[-4\sigma_e;4\sigma_e\right]$, and we presume for simplicity a Gaussian distribution of angles for the calculation of the weighted concentration average. The 'external' wind-angle variability σ_e is estimated from Eq. (1), with a zero lower bound, where σ_α is obtained from the Prairie Grass experiments, and where σ_m can be obtained by applying the level 2 model of Mellor and Yamada (1982) to the surface layer of the atmospheric boundary layer, resulting in

$$\langle u\rangle^2\sigma_m^2 = \langle v^2\rangle \approx \gamma_1\left(\frac{u_*}{\phi_M S_M}\right)^2, \tag{10}$$

with S_M given by

$$S_M = \left(\frac{\phi_M^{-4}}{B_1(1-R_f)}\right)^{1/3}, \tag{11}$$

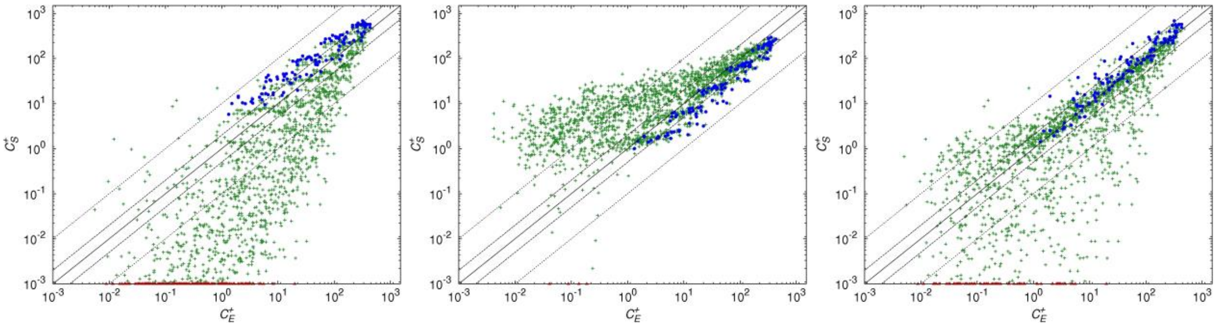
and with $\gamma_1 \approx 0.22$ and $B_1 \approx 16.6$, two empirical constants (Mellor and Yamada, 1982).

Finally, in order to assess the quality of the approach, we use a set of performance criteria proposed by Chang and Hanna (2004), i.e. the fraction bias (FB), the geometric mean bias (MG), the normalized mean square error (NMSE), the geometric variance (VG), and the fraction of predictions within a factor of two of observations (FAC2). Additionally, although not a part of the performance criteria of Chang and Hanna (2004), we will also look at FAC10, defined similar to FAC2. Remark that all measurement points are taken into account i.e. without imposing a concentration threshold, following a paired-in-space approach.

RESULTS AND DISCUSSION

In the current section, we briefly present the results of the proposed extension of the approach discussed in Vervecken et al. 2013 to include thermal stratification in RANS simulation in addition to including the variable wind direction, using the estimated 'external' wind-angle variability σ_e ('σ_e-RANS'). For comparison, we also add results obtained using two other models: (1) RANS simulations using the mean-wind direction only ('mean-wind RANS'), and (2) RANS simulations using the total wind variability ('σ_α-RANS').

In figure 1, a scatter plot is provided for the three models studied, that displays the value of the model predictions versus the corresponding experimental observations in case of stable stratification. In these graphs, points plotted using a solid circle represent the arc centreline concentrations while the crosses represent all other measurements. The solid triangles on abscissa indicate predicted concentrations falling below the range of the graph. First of all, it is observed in that the 'mean-wind RANS' simulations (Fig.1a) systematically overestimate the centreline concentrations while the opposite is observed for the 'σ_α-RANS' simulations (Fig.1b). In case of the 'σ_e-RANS' simulations (Fig.1c) however, the centreline concentrations are well reproduced with only a few predictions off by more than a factor of two.



(a) (b) (c)

Figure 1. Scatter plot of the simulated versus experimentally observed concentrations (C_s^+ versus C_E^+) at observation arcs and towers under stable stratification. Symbols: (●): centreline concentrations; (▲): simulation results with $C_s^+ < 10^{-3}$; (+) all other points. Lines: (−) $C_s^+ = C_E^+$; (--): $C_s^+ = 2^{\pm1}C_E^+$; (…): $C_s^+ = 10^{\pm1}C_E^+$. (a) 'mean-wind RANS', (b) 'σ_α-RANS', (c) 'σ_e-RANS'.

When taking the off-centreline measurements into account, the ‘mean-wind RANS’ model underestimates the majority of the low concentrations measured, and many of them by several orders of magnitude, as opposed to the ‘σ_α-RANS’ approach that shows a clear bias towards overestimating these concentrations. The ‘σ_e-RANS’ approach falls between the two other models, improving the prediction of both high and low concentrations.

To quantitatively evaluate the modelling approach, an evaluation of the performance criteria following Chang and Hanna (2004) is given in Table 1 for the centreline concentrations and all measurements, respectively. With respect to the centreline concentrations, the ‘σ_e-RANS’ approach performs markedly better than the two other models, meeting all performance measures regardless the thermal stratification. The ‘σ_α-RANS’ approach shows a systematic bias towards underestimating the centerline concentrations while the ‘mean-wind RANS’ is overly conservative. When taking the off-centreline measurements into account, the ‘mean-wind RANS’ approach again performs the worst, mainly due to the large number of strongly underestimated concentrations, e.g. with MG and VG virtually infinite as a result. The ‘σ_e-RANS’ and ‘σ_α-RANS’ performance measures are comparable but the ‘σ_e-RANS’ approach are closer to the optimal value. Finally note that under strong stable stratification, the external variability σ_e (cf. Eq. 1) becomes negligible with respect to modelled σ_m i.e. ‘σ_e-RANS’ converges towards ‘mean-wind RANS’. Under strong unstable stratification on the other hand, the modeled variability σ_m (cf. Eq. 1) becomes negligible with respect to σ_e and ‘σ_e-RANS’ converges towards ‘σ_α-RANS’.

CONCLUSION

In the current work, we extend the approach presented in Vervecken et al. (2013), which incorporates the wind variability in the simulation taking into account the variability represented by the RANS turbulence model, towards thermally stratified boundary layers by application of the Monin-Obukhov similarity theory. We test the extended approach by performing a series of dispersion simulations of the Project Prairie Grass experiments and compare the results with two other models by evaluating the model performance criteria of Chang and Hanna (2004). We found that the extended model is well capable of reproducing the centreline concentrations, meeting the model performance criteria regardless the stratification. When taking the off-centreline measurements into account, the model reproduces the high concentrations without a significant bias or scatter and improves the prediction of the lower concentrations compared to the ‘mean-wind RANS’ and ‘σ_α-RANS’ simulations.

Table 1. Comparison of statistical performance measures computed based on both centreline concentrations and all measurements of the models applied to the Prairie Grass experiments under unstable (6 experiments, 1066 measurements), neutral (21 experiments, 2899 measurements) and stable (24 experiments, 1841 measurements) thermal stratification. The values closest to the optimal value are indicated in bold. Performance measures that fall within the acceptance limits set by Chang and Hanna (2004) are highlighted.

			FB	**MG**	**NMSE**	**VG**	**FAC2**	**FAC10**
			-0.3 < FB < 0.3	0.7 < MG < 1.3	< 4	< 1.6	> 0.5	-
Centreline measurements	unstable	mean-wind RANS	-1.295	0.104	6.483	168.7	0.000	0.500
		σ_α-RANS model	0.356	**0.889**	1.148	**1.014**	**0.767**	**0.967**
		σ_e-RANS model	**0.293**	0.835	**0.968**	1.033	**0.767**	**0.967**
	neutral	mean-wind RANS	-1.176	0.150	4.446	36.73	0.010	0.750
		σ_α-RANS model	0.190	**0.931**	0.349	**1.005**	**0.875**	**1.000**
		σ_e-RANS model	**0.004**	0.781	**0.196**	1.063	0.837	**1.000**
	stable	mean-wind RANS	-0.569	0.444	0.786	1.931	0.436	**1.000**
		σ_α-RANS model	0.518	1.904	0.691	1.514	0.615	**1.000**
		σ_e-RANS model	**-0.264**	**0.757**	**0.349**	**1.080**	**0.855**	**1.000**
All measurements	unstable	mean-wind RANS	0.043	Inf	11.559	Inf	0.069	0.216
		σ_α-RANS model	0.101	0.464	1.210	1.802	**0.526**	0.873
		σ_e-RANS model	**0.093**	**0.491**	**1.090**	**1.658**	**0.526**	**0.878**
	neutral	mean-wind RANS	-0.029	Inf	7.891	Inf	0.080	0.271
		σ_α-RANS model	0.007	0.521	0.484	1.530	**0.639**	0.896
		σ_e-RANS model	**-0.006**	**0.638**	**0.371**	**1.224**	0.616	**0.918**
	stable	mean-wind RANS	0.117	Inf	1.626	Inf	0.205	0.447
		σ_α-RANS model	0.142	**0.339**	0.913	**3.213**	0.442	**0.750**
		σ_e-RANS model	**0.112**	Inf	**0.742**	Inf	**0.483**	0.738

REFERENCES

Barad, M.L., 1958: Project Prairie Grass, A Field Program in Diffusion. *Geophysical Research Papers* No. 59, vols. I and II. Air Force Cambridge Research Center. Rep. Technical Report. AFCRC-TR-58-235.

Bird, R., W. Stewart and E. Lightfoot, 2006: Transport Phenomena, Wiley, 995 pp.

Blocken, B., T. Stathopoulos, P. Saathoff and X. Wang, 2008: Numerical evaluation of pollutant dispersion in the built environment: Comparisons between models and experiments. *Journal of Wind Engineering and Industrial Aerodynamics*, **96**, 1817-1831.

Brunel, J.P., 1989: Estimation of sensible heat flux from measurements of surface radiative temperature and air temperature at two meters: application to determine actual evaporation rate. *Agricultural and Forest Meteorology*, **46**, 179-191.

Businger, J.A., J.C. Wyngaard, Y. Izumi and E.F. Bradley, 1971: Flux-Profile Relationships in the Atmospheric Surface Layer. *J. Atmos. Sci.*, **28**, 181–189.

Chang, J.C. and S.R. Hanna, 2004: Air quality model performance evaluation. *Meteorology and Atmospheric Physics*, **87**, 167-196.

Dyer A.J., 1974: A review of flux-profile relationships, *Boundary Layer Meteorol.*, **20**, 35–49.

Foken, T. , 2006: 50 Years of the Monin–Obukhov Similarity Theory. *Boundary-Layer Meteorology*, **119**(3), 431-447.

Garrat J. and R.A. Pielke, 1989: On the sensitivity of Mesoscale Models to surface-layer parameterization constants. *Boundary-Layer Meteorol.*, **48**, 377-387.

Huber, A., W. Tang, A. Flowe, B. Bell, K. Kuehlert and W. Schwarz, 2004: Development and applications of CFD simulations in support of air quality studies involving buildings. *Proceedings of 13th joint conference on the applications of air pollution meteorology with the Air & Waste Management Association.* Vancouver, British Columbia, Canada.

Mellor, G.L. and T. Yamada, 1982: Development of a turbulence closure model for geophysical fluid problems. *Reviews of geophysics and space physics*, **20**(4), 851-875.

Monin, A.S. and A. Obukhov, 1954: Basic laws of turbulent mixing in the surface layer of the atmosphere. *Trudy Geofiz. Inst. Acad. Nauk SSSR*, **24**(151), 163-187.

Paulson, C.A., 1970: The mathematical representation of wind speed and temperature profiles in the unstable atmospheric surface layer. *J. Appl.Meteor.*, **9**, 857–861.

Piringer, M. and K. Baumann-Stanzer, 2009: Selected results of a model validation exercise. *Advances in Science and Research* **3**, 13–16.

Riddle, A., D. Carruthers, A. Sharpe, C. McHugh and J. Stocker, 2004: Comparisons between FLUENT and ADMS for atmospheric dispersion modelling. *Atmospheric environment*, **38**(7), 1029-1038.

Stull, R.B., 1988: An introduction to boundary layer meteorology, Vol. 13, Kluwer Academic Pub, 666 pp.

Tennekes, H. and J.L. Lumley, 1972: A first Course in Turbulence, The MIT Press, 300 pp.

Tang, W., A. Huber, B. Bell and W. Schwartz, 2006: Application of CFD Simulations for Short-Range Atmospheric Dispersion, *14th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Assoc*.

Thoman, D. C., K.R. O'Kula, J.C. Laul, M.W. Davis and K.D. Knecht, 2006: Comparison of ALOHA and EPIcode for Safety Analysis Applications. *Journal of Chemical Health and Safety*, **13**(6), 20-33.

Tominaga, Y. and T. Stathopoulos, 2007: Turbulent Schmidt numbers for CFD analysis with various types of flowfield. *Atmospheric Environment*, **41**, 8091-8099.

Vervecken, L., J. Camps and J. Meyers, 2013: Accounting for wind-direction fluctuations in Reynolds-averaged simulation of near-range atmospheric dispersion. *Atmospheric Environment*, **72**, 142-150, doi:10.1016/j.atmosenv.2013.03.005 .

Zannetti, P., 1990: Air Pollution Modeling. Theories, Computational Methods and Available Software. Computational Mechanics Publications, 444 pp.